

chain nodes :
8 15 16 17 18 22 23 24 25 27 28 29
ring nodes :
1 2 3 4 5 6 9 10 11 12 13 14
chain bonds :
5-8 14-15 15-16 16-22 16-23 22-24 23-28 23-29 24-25 24-27
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 9-10 9-14 10-11 11-12 12-13 13-14
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-8 16-22 22-24 23-28 23-29 24-25 24-27
exact bonds :
14-15 15-16 16-23
normalized bonds :
9-10 9-14 10-11 11-12 12-13 13-14
isolated ring systems :
containing 1 : 9 :

G1:O,S
G2:[*1],[*2]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:CLASS 16:CLASS 17:CLASS 18:CLASS 22:CLASS 23:CLASS
24:CLASS 25:CLASS 27:Atom 28:CLASS 29:CLASS 31:CLASS

* * * * * Welcome to STN International * * * * *

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
 NEWS 2 "Ask CAS" for self-help around the clock
 NEWS 3 May 10 PROUSDDR now available on STN
 NEWS 4 May 19 PROUSDDR: One FREE connect hour, per account, in both May
 and June 2004
 NEWS 5 May 12 EXTEND option available in structure searching
 NEWS 6 May 12 Polymer links for the POLYLINK command completed in REGISTRY
 NEWS 7 May 17 FRFULL now available on STN
 NEWS 8 May 27 New UPM (Update Code Maximum) field for more efficient patent
 SDIs in CAPLUS
 NEWS 9 May 27 CAPLUS super roles and document types searchable in REGISTRY
 NEWS 10 May 27 Explore APOLLIT with free connect time in June 2004
 NEWS 11 Jun 22 STN Patent Forums to be held July 19-22, 2004

NEWS EXPRESS MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT
 MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
 AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004
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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 15:53:31 ON 23 JUN 2004

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

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Property values tagged with IC are from the ZIC/VINITI data file
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STRUCTURE FILE UPDATES: 22 JUN 2004 HIGHEST RN 697737-72-7

DICTIONARY FILE UPDATES: 22 JUN 2004 HIGHEST RN 697737-72-7

TS/CA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when
 conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

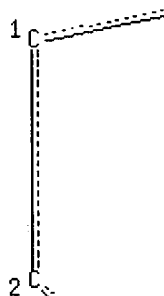
L1 STRUCTURE UPLOADED

=> d l1

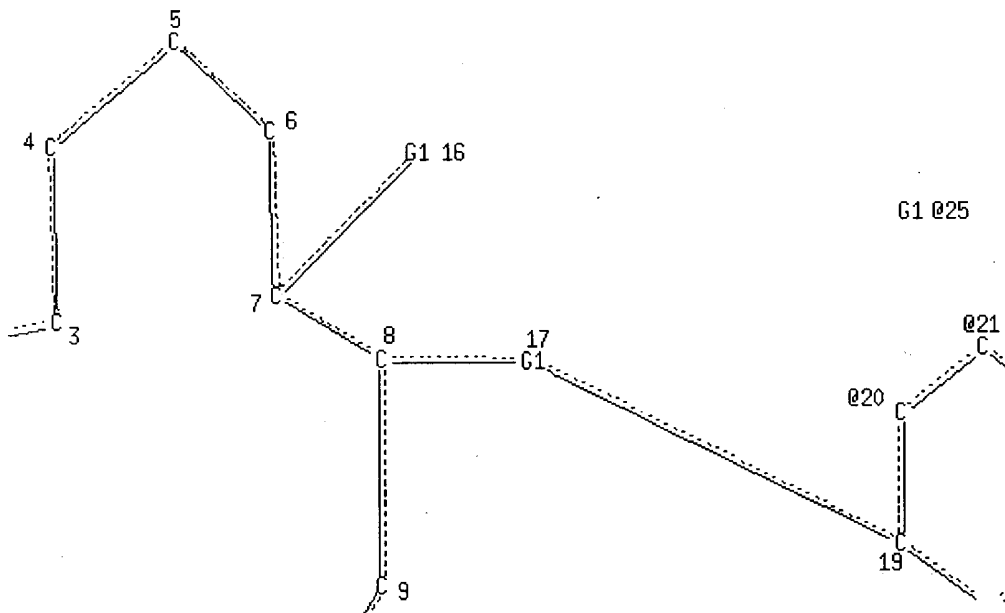
L1 HAS NO ANSWERS

L1 STR

0 29 S 30

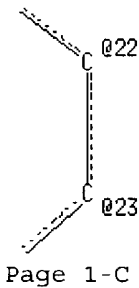


Page 1-A

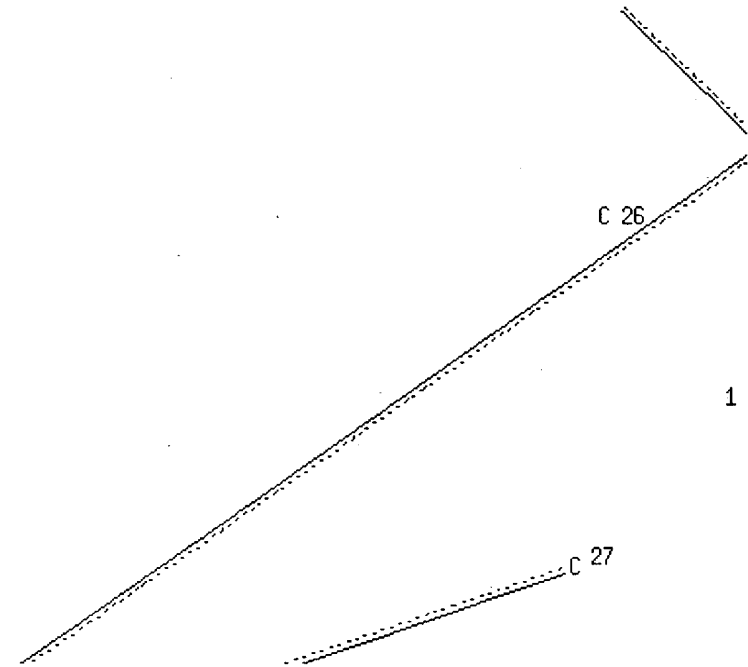


Page 1-B

N 024

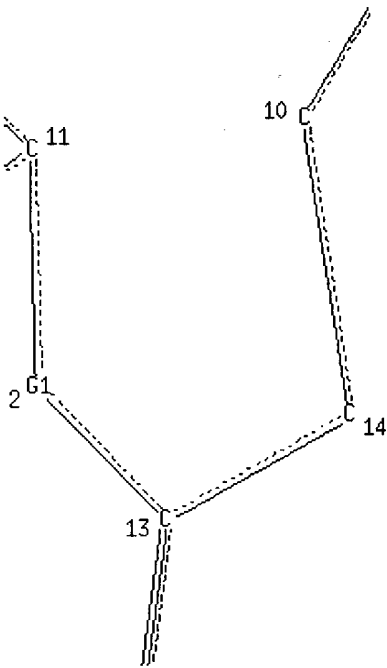


Page 1-C



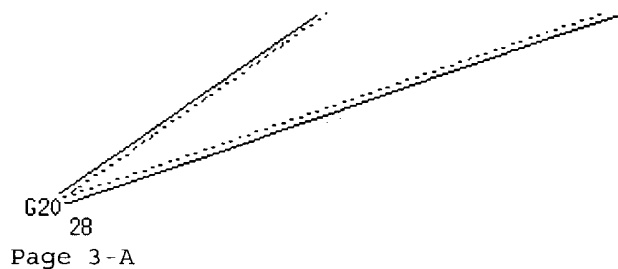
Page 2-A

C1
18



Page 2-B

Page 2-C



Page 3-B

VAR G1=29/30

REP G20=(0-2) 26-11 26-27

VPA 24-20/21/22/23 S

VPA 25-20/21/22/23 S

NODE ATTRIBUTES:

NSPEC	IS R	AT	1
NSPEC	IS R	AT	2
NSPEC	IS R	AT	3
NSPEC	IS R	AT	4
NSPEC	IS R	AT	5
NSPEC	IS R	AT	6
NSPEC	IS R	AT	7
NSPEC	IS R	AT	8
NSPEC	IS R	AT	9
NSPEC	IS R	AT	10
NSPEC	IS R	AT	11
NSPEC	IS R	AT	12
NSPEC	IS R	AT	13
NSPEC	IS R	AT	14
NSPEC	IS C	AT	15
NSPEC	IS C	AT	16
NSPEC	IS C	AT	17
NSPEC	IS R	AT	18
NSPEC	IS R	AT	19
NSPEC	IS R	AT	20
NSPEC	IS R	AT	21
NSPEC	IS R	AT	22
NSPEC	IS R	AT	23
NSPEC	IS C	AT	24
NSPEC	IS C	AT	25
NSPEC	IS C	AT	26
NSPEC	IS C	AT	27
NSPEC	IS C	AT	28

DEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 24 26 27

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 30

STEREO ATTRIBUTES: NONE

=> s 11

SAMPLE SEARCH INITIATED 15:56:48 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 6851 TO ITERATE

14.6% PROCESSED 1000 ITERATIONS 40 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 132059 TO 141981
PROJECTED ANSWERS: 4487 TO 6473

L2 40 SEA SSS SAM L1

=>

L3 STRUCTURE UPLOADED

=> d 13

L3 HAS NO ANSWERS

L3 STR

=> s 13

SAMPLE SEARCH INITIATED 16:00:20 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 4369 TO ITERATE

22.9% PROCESSED 1000 ITERATIONS 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 83417 TO 91343
PROJECTED ANSWERS: 3719 TO 5543

L4 50 SEA SSS SAM L3

=>

L5 STRUCTURE UPLOADED

=> 15

L5 IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

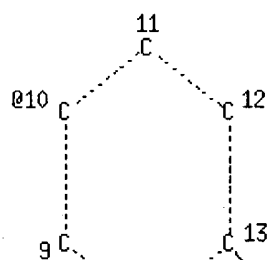
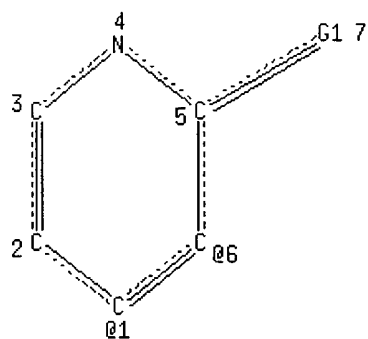
=> d 15

L5 HAS NO ANSWERS

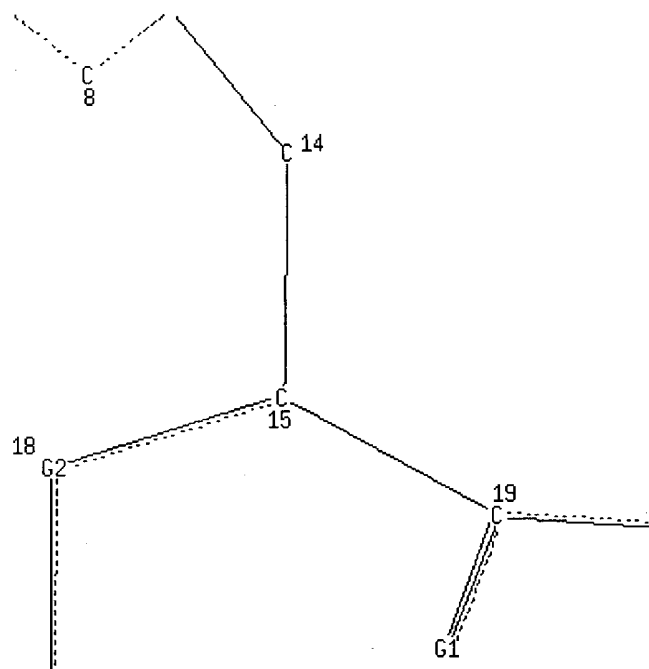
L5 STR

0 25 S 26

Page 1-A



Page 1-B



Page 2-B

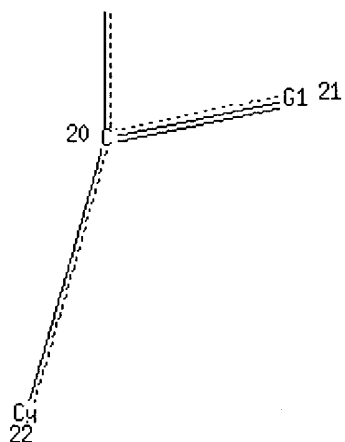
---G2 24

Page 2-C

N 17

Page 3-A

23



Page 3-B

0 16

Page 4-A

VAR G1=25/26

VAR G2=16/17

VPA 10-1/6 S

NODE ATTRIBUTES:

NSPEC	IS R	AT	1
NSPEC	IS R	AT	2
NSPEC	IS R	AT	3
NSPEC	IS R	AT	4
NSPEC	IS R	AT	5
NSPEC	IS R	AT	6
NSPEC	IS C	AT	7
NSPEC	IS R	AT	8
NSPEC	IS R	AT	9
NSPEC	IS R	AT	10
NSPEC	IS R	AT	11
NSPEC	IS R	AT	12
NSPEC	IS R	AT	13
NSPEC	IS C	AT	14
NSPEC	IS C	AT	15
NSPEC	IS C	AT	16
NSPEC	IS C	AT	17
NSPEC	IS C	AT	18
NSPEC	IS C	AT	19
NSPEC	IS C	AT	20
NSPEC	IS C	AT	21
NSPEC	IS C	AT	22
NSPEC	IS C	AT	23
NSPEC	IS C	AT	24

DEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 14 15 16 17 19 20 25 26

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 26

STEREO ATTRIBUTES: NONE

=> s 15

SAMPLE SEARCH INITIATED 16:11:32 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 733 TO ITERATE

100.0% PROCESSED 733 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 13036 TO 16284
PROJECTED ANSWERS: 2 TO 124

L6 2 SEA SSS SAM L5

=> s 15 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 16:11:36 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 14388 TO ITERATE

100.0% PROCESSED 14388 ITERATIONS 42 ANSWERS
SEARCH TIME: 00.00.01

L7 42 SEA SSS FUL L5

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	167.60	167.81

FILE 'HCAPLUS' ENTERED AT 16:11:40 ON 23 JUN 2004
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FILE COVERS 1907 - 23 Jun 2004 VOL 140 ISS 26
FILE LAST UPDATED: 22 Jun 2004 (20040622/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 17

L8 2 L7

=> s 18 and kaplan, g?/au

348 KAPLAN, G?/AU

L9 1 L8 AND KAPLAN, G?/AU

=> d 19, ibib abs fhitr, 1

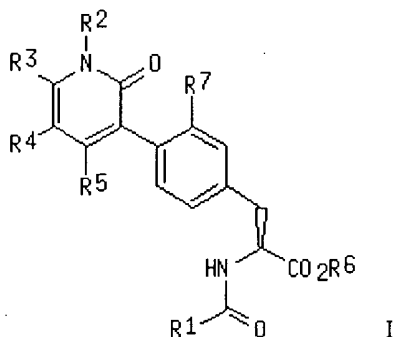
L9 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
--------------	----------------------

ACCESSION NUMBER: 2001:435046 HCAPLUS
 DOCUMENT NUMBER: 135:33647
 TITLE: Preparation of pyridinyl phenylalanine derivatives
 INVENTOR(S): Kaplan, Gerald Lewis; Sidduri, Achyutharao; Tilley, Jefferson Wright
 PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.
 SOURCE: PCT Int. Appl., 97 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001042215	A1	20010614	WO 2000-EP11979	20001129
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6388084	B1	20020514	US 2000-717684	20001121
BR 2000016172	A	20020820	BR 2000-16172	20001129
EP 1244625	A1	20021002	EP 2000-985117	20001129
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003516392	T2	20030513	JP 2001-543516	20001129
NZ 518888	A	20040227	NZ 2000-518888	20001129
US 2002133015	A1	20020919	US 2002-59618	20020129
NO 2002002650	A	20020605	NO 2002-2650	20020605
PRIORITY APPLN. INFO.:				
			US 1999-169090P	P 19991206
			US 2000-245603P	P 20001103
			US 2000-717684	A3 20001121
			WO 2000-EP11979	W. 20001129

OTHER SOURCE(S): MARPAT 135:33647
 GI



AB Pyridinyl phenylalanine derivs. I (R1 = substituted aryl, substituted 5 or 6 membered heteroarom. ring contg. N, O and S bonded via a carbon atom to

the amide carbonyl, 3-7 membered ring substituted with alkyl, alkenyl, fluorinealkenyl, arylalkyl, heteroarylalkyl, azidoalkyl, cyanoalkyl, hydroxyalkyl, alkyl sulfonyl, alkyl sulfinyl; R2 = H, (un)substituted alkyl, aryl, or arylalkyl; R3 = H, halogen, alkyl, trifluoromethyl, or aryl; R4 = H, halogen, alkyl, or aryl; R5 = H, alkyl, alkoxy, trifluoromethyl, or aryl; R6 = H, alkyl, alkylcarbonyloxy, substituted aminoalkyl, substituted heterocyclalkyl; R7 = H, Cl, alkoxy, or alkyl) were prepd. as inhibitors of the binding of VCAM-1 to VLA-4 and are useful in treating chronic inflammatory diseases. Thus, N-[(2-chloro-6-methylphenyl)carbonyl]-4-(5-chloro-1-methyl-2-oxo-3-pyridinyl)-L-phenylalanine (II) was prepd. from N-[(1,1-dimethylethoxy)carbonyl]-4-iodo-L-phenylalanine Me ester in 5 steps via palladium catalyzed reaction with 3-bromo-5-chloro-1-methyl-2-pyridinone and coupling with 2-chloro-6-methylbenzoic acid. II showed antiinflammatory activity in vitro in the VCAM/VLA-4 screening assay (IC50 < 1 nM).

IT **343981-05-5P**

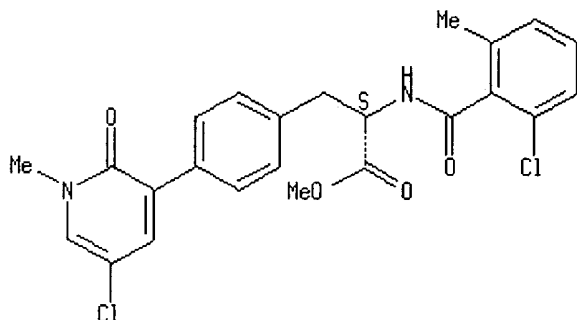
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. of pyridinyl phenylalanine derivs. as anti-inflammatory agents)

RN **343981-05-5** HCAPLUS

CN L-Phenylalanine, 4-(5-chloro-1,2-dihydro-1-methyl-2-oxo-3-pyridinyl)-N-(2-chloro-6-methylbenzoyl)-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 15:53:31 ON 23 JUN 2004)

FILE 'REGISTRY' ENTERED AT 15:53:37 ON 23 JUN 2004

L1 STRUCTURE UPLOADED
L2 40 S L1
L3 STRUCTURE UPLOADED
L4 50 S L3
L5 STRUCTURE UPLOADED
L6 2 S L5
L7 42 S L5 FULL

FILE 'HCAPLUS' ENTERED AT 16:11:40 ON 23 JUN 2004

L8 2 S L7
L9 1 S L8 AND KAPLAN, G?/AU

```
=> s 12 not 19
      62 L2
L10    62 L2 NOT L9

=> s 18 not 19
L11    1 L8 NOT L9

=> s 111 and sidduri, a?/au
      18 SIDDURI, A?/AU
L12    0 L11 AND SIDDURI, A?/AU

=> s 111 and tilley, j?/au
      171 TILLEY, J?/AU
L13    0 L11 AND TILLEY, J?/AU

=>
```